



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:07 PM UTC

PDB ID : 2AHB / pdb_00002ahb
Title : X-ray crystal structure of R46A,R161A mutant of Mycobacterium tuberculosis FabH
Authors : Brown, A.K.; Sridharan, S.; Kremer, L.; Lindenberg, S.; Dover, L.G.; Sacchetti, J.C.; Besra, G.S.
Deposited on : 2005-07-27
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

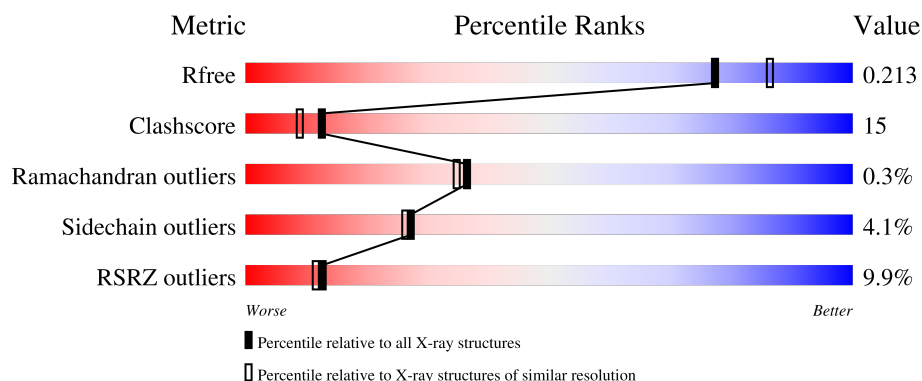
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5097 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta- ketoacyl-ACP synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2430	1518	426	472	14			
1	B	334	Total	C	N	O	S	0	0	0
			2430	1518	426	472	14			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	cloning artifact	UNP P0A574
A	-19	GLY	-	cloning artifact	UNP P0A574
A					

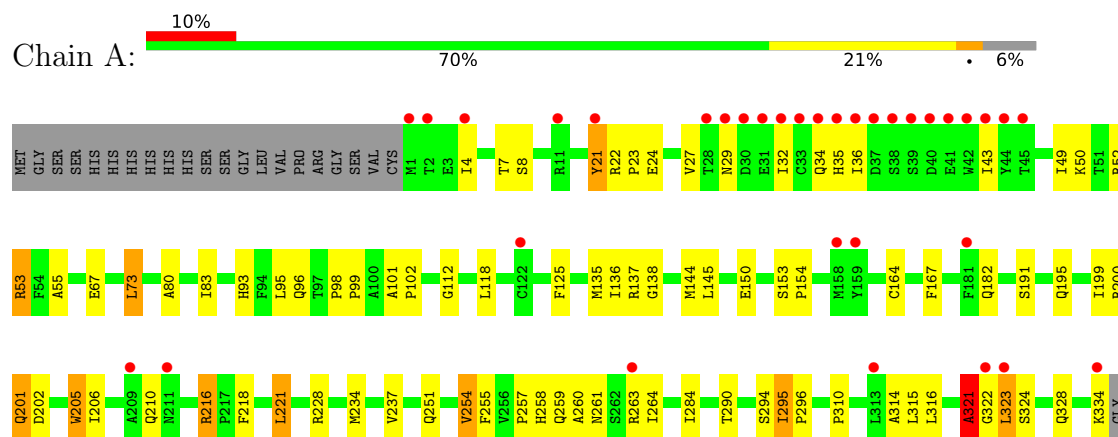
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	cloning artifact	UNP P0A574
B	-17	SER	-	cloning artifact	UNP P0A574
B	-16	HIS	-	expression tag	UNP P0A574
B	-15	HIS	-	expression tag	UNP P0A574
B	-14	HIS	-	expression tag	UNP P0A574
B	-13	HIS	-	expression tag	UNP P0A574
B	-12	HIS	-	expression tag	UNP P0A574
B	-11	HIS	-	expression tag	UNP P0A574
B	-10	SER	-	cloning artifact	UNP P0A574
B	-9	SER	-	cloning artifact	UNP P0A574
B	-8	GLY	-	cloning artifact	UNP P0A574
B	-7	LEU	-	cloning artifact	UNP P0A574
B	-6	VAL	-	cloning artifact	UNP P0A574
B	-5	PRO	-	cloning artifact	UNP P0A574
B	-4	ARG	-	cloning artifact	UNP P0A574
B	-3	GLY	-	cloning artifact	UNP P0A574
B	-2	SER	-	cloning artifact	UNP P0A574
B	-1	VAL	-	cloning artifact	UN

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta- ketoacyl-ACP synthase III



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.44Å 81.41Å 97.28Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 99.4 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.248 0.222 , 0.213	Depositor DCC
R_{free} test set	2586 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2474	0.95	11/3367 (0.3%)
1	B	0.41	0/2474	0.97	13/3367 (0.4%)
All	All	0.41	0/4948	0.96	24/6734 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LYS	N-CA-C	5.30	120.40	113.88
1	A	93	HIS	N-CA-C	-5.27	98.72	107.99
1	B	202	ASP	N-CA-C	5.21	117.86	111.82
1	B	294	SER	N-CA-C	5.20	116.63	111.07
1	A	24	GLU	N-CA-C	5.19	116.63	111.07
1	B	112	GLY	N-CA-C	5.17	122.25	115.47
1	A	205	TRP	N-CA-C	5.13	117.61	111.71
1	B	167	PHE	N-CA-C	5.13	118.08	110.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	LEU	Mainchain

5.2 Too-close contacts [i](#)

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:CB	1:B:323:LEU:HD22	2.08	0.84
1:B:261:ASN:HD22	1:B:264:ILE:H	1.24	0.83
1:A:135:MET:HB3	1:A:144:MET:HE1	1.63	0.81
1:A:234:MET:HA	1:A:237:VAL:HG12	1.63	0.81
1:A:261:ASN:HD22	1:A:264:ILE:H	1.26	0.80
1:B:321:ALA:C	1:B:323:LEU:H	1.88	0.79
1:A:205:TRP:HE1	1:B:96:GLN:HE21	1.33	0.77
1:B:227:PHE:HB3	1:B:264:ILE:HD11	1.68	0.76
1:A:80:ALA:HA	1:A:83:ILE:HD12	1.72	0.72
1:A:321:ALA:C	1:A:323:LEU:H	1.97	0.72
1:A:295:ILE:HD11	1:A:316:LEU:HD13	1.72	0.71
1:B:199:ILE:HG12	1:B:221:LEU:CD2	2.23	0.69
1:B:100:ALA:HA	1:B:103:MET:HE3	1.75	0.68
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.58	0.67
1:A:73:LEU:HD11	1:A:83:ILE:HD11</		

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:CD1	1:A:316:LEU:HD13	2.33	0.59
1:B:15:LEU:HG	1:B:184:ILE:HD11	1.85	0.59
1:B:47:THR:HG21	1:B:165:PHE:HE2	1.67	0.58
1:B:14:GLY:HA2	1:B:184:ILE:HG12	1.86	0.58
1:A:234:MET:HA	1:A:237:VAL:CG1	2.32	0.58
1:B:265:ASN:O	1:B:269:VAL:HG23	2.04	0.57
1:B:35:HIS:HB3	1:B:159:TYR:CE1	2.39	0.57
1:B:195:GLN:HB3	1:B:323:LEU:HD22	1.84	0.57
1:A:136:ILE:HG13	1:A:144:MET:HE2	1.86	0.57
1:B:69:CYS:O	1:B:73:LEU:HD13	2.06	0.56
1:B:252:ILE:HD12	1:B:252:ILE:N	2.20	0.56
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.89	0.55
1:A:4:ILE:HD11	1:B:313:LEU:CD1	2.32	0.55
1:B:261:ASN:ND2	1:B:264:ILE:H	2.01	0.55
1:A:8:SER:HB3	1:B:11		

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG13	1:A:314:ALA:CB	2.41	0.50
1:A:205:TRP:NE1	1:B:96:GLN:HE21	2.05	0.50
1:B:155:THR:O	1:B:219:VAL:HG12	2.12	0.50
1:B:320:GLY:O	1:B:323:LEU:HA	2.12	0.50
1:A:8:SER:HB3	1:B:11:ARG:NH2	2.26	0.49
1:A:96:GLN:HG2	1:B:201:GLN:HE22	1.77	0.49
1:B:206:ILE:O	1:B:210:GLN:HG3	2.12	0.49
1:A:136:ILE:HG13	1:A:144:MET:HE3	1.95	0.49
1:B:122:CYS:HB2	1:B:320:GLY:HA3	1.94	0.49
1:B:211:ASN:N	1:B:212:PRO:HD3	2.26	0.49
1:A:49:ILE:HG12	1:A:284:ILE:HG12	1.93	0.49
1:B:27:VAL:HG11	1:B:32:ILE:HD11	1.94	0.49
1:B:111:LYS:HA	2:B:510:HOH:O	2.12	0.49
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.96	0.48
1:B:188:VAL:HG			

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:HB3	1:B:91:ASN:O	2.19	0.42
1:A:254:VAL:CG1	1:A:314:ALA:HB2	2.48	0.42
1:A:228:ARG:HH11	1:A:228:ARG:HG2	1.85	0.42
1:B:23:PRO:HG2	1:B:53:ARG:CB	2.49	0.42
1:B:163:ASN:C	1:B:163:ASN:HD22	2.27	0.42
1:A:261:ASN:ND2	1:A:263:ARG:N	2.68	0.42
1:A:263:ARG:HH11	1:A:263:ARG:HG3	1.86	0.41
1:A:216:ARG:HD2	1:A:218:PHE:CZ	2.54	0.41
1:A:234:MET:C	1:A:237:VAL:HG12	2.45	0.41
1:A:73:LEU:HD11	1:A:83:ILE:CD1	2.49	0.41
1:B:268:LEU:O	1:B:272:LEU:HB2	2.21	0.41
1:B:49:ILE:HG12	1:B:284:ILE:HG12	2.03	0.41
1:B:89:THR:HA	1:B:118:LEU:O	2.21	0.41
1:A:191:SER:HA	1:A:324:SER:HA	2.02	0.41
1:A:295:ILE:HD13			

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	ALA
1	A	321	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/262 (93%)	232 (95%)	12 (5%)	22	20
1	B	244/262 (93%)	236 (97%)	8 (3%)	33	34
All	All	488/524 (93%)	468 (96%)	20 (4%)	27	26

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	53	ARG
1	A	73	LEU
1	A	95	LEU
1	A	118	LEU
1	A		

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	75	ASN
1	A	182	GLN
1	A	201	GLN
1	A	258	HIS
1	A	261	ASN
1	A	265	ASN
1	B	34	GLN
1	B	75	ASN
1	B	91	ASN
1	B	93	HIS
1	B	96	GLN
1	B	163	ASN
1	B	201	GLN
1	B	211	ASN
1	B	261	ASN
1	B	265	ASN
1	B	273	GLN
1	B	286	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Lig

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	334/356 (93%)	0.53	34 (10%)	12 11	16, 31, 59, 84	0
1	B	334/356 (93%)	0.59	32 (9%)	13 12	16, 30, 53, 90	0
All	All	668/712 (93%)	0.56	66 (9%)	13 11	16, 30, 58, 90	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	CYS	11.0
1	B	38	SER	9.5
1	A			

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Mol	Chain	Res	Type	RSRZ
1	A	29	ASN	3.3
1	A	263	ARG	3.3
1	A	28	THR	3.3
1	B	21	TYR	3.3
1	A	30	ASP	3.3
1	B	3	GLU	3.3
1	A	334	LYS	3.3
1	B	334	LYS	3.2
1	B	30	ASP	3.1
1	B	111	LYS	3.0
1	B	37	ASP	2.9
1	B	179	THR	2.9
1	B	323	LEU	2.9
1	A	40	ASP	2.8
1	A	21	TYR	2.8
1	B	12	SER	2.7
1	B	11	ARG	2.7
1	A	34	GLN	2.7
1	B	159	TYR	2.7
1	A	39	SER	2.7
1	A	211	ASN	2.7
1	A	4	ILE	2.7
1	B	43	ILE	2.6
1	B	161	ALA	2.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.